KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2017/2018 ACADEMIC YEAR

FOURTH YEAR SECOND SEMESTER
MAIN EXAMINATIONS

FOR THE DEGREE OF SCIENCE

COURSE CODE: SCH 411

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 2 HOURS

DATE: 30/7/2018 TIME: 2-4PM

INSTRUCTIONS TO CANDIDATES

- Answer **QUESTION ONE** (Compulsory) and any other two (2) Questions.
- Indicate **answered questions** on the front cover.
- Start every question on a new page and make sure question's number is written on each page.
- You are provided with graph papers where necessary.

This paper consists of 4 printed pages. Please Turn Over

Useful Information

$R = 8.314\ JK^{-1}\ mol^{-1}$ or $0.08206\ L\ atm\ K^{-1}\ mol^{-1}$

$1\ atm = 1.01325\ bar = 760\ torr = 1.01325 \times 10^5\ Pa = 760mmHg$

$e = 1.60217662 \times 10^{-19}\ C$

$IJ = CV = lKgm^2s^{-2}$

$h = 6.626xl0^{-34}Js$

$N_A = 6.022\ X10^{23}$ /molecules

QUESTION ONE (30MARKS)

a) Define the following terms as used in quantum chemistry **[4 marks]**

i. Wave-function
ii. Photo electric effect
iii. Wave-particle duality
iv. Nodes

b) Explain what is meant by Ritz Combination principle **[3 marks]**

c) Calculate the uncertainty in position of an electron if the uncertainty in velocity is $5.7 \times 10^5 m\ sec^{-1}$ **[5 marks]**

d) Calculate the wavelength in A^0 of the line with n=3 in the Balmer series of the spectrum of atomic hydrogen. **[4 marks]**

e) Calculate the ionization energy Ei for hydrogen like atom of H, He^+, Li^{2+} and Be whose Ei=13.606eV **[4 marks]**

f) What is the ground state energy for an election that is confined to a potential well with a width of 0.2 nm? **[5 marks]**

g) What is the de-Broglie wavelength I of an electron that has been accelerated through a potential difference of 100v **[3 marks]**

State two basic principle of classical mechanic

h) State two basic principle of classical mechanic **[2 marks]**

QUESTION TWO (20 M A R K S)

a) Show that $m \frac{d^2x}{d^2} + kx = 0$ also applies to mass m_1 connected to mass m_2 by a **[4 marks]** spring exhibiting harmonic motion.

b) i. Derive the Schrödinger Wave Equation as used in quantum chemistry **[10marks]**
ii. State four characteristics of the Schrödinger Wave Equation **[4marks]**
iii. Explain the meaning of ψ^2 **[2marks]**

QUESTION THREE (20MARKS)

a) Normalize the molecular orbital $\Psi = N(A-B)$ state the meaning of the overlap integral S in this probability of this wavefunction. **[5 marks]**

b) How many electrons can enter the following sets of atomic orbitals: 1s,2s, 3s, 3p, and 3d **[3 marks]**

c) Explain the six postulates of quantum mechanics **[12marks]**

QUESTION FOUR (20M A R KS)

a) Explain two reasons why zero point energy must exist **[3 marks]**

b) What is Compton Effect **[2 marks]**

c) What are the reduced mass and moment of inertia of HCL? The equilibrium internuclear distance R_e is 127.5 pm. What are the values of L1, Lz and E for the state with J = I? Atomic masses of s of H $=1.007825X10^{-3}Kgmol^{-1}$ and Cl^{35} $34.96885x10^{-3}kgmol^{-1}$ and $h=1.054x10^{-34}js$ **[10 marks]**

d) Derive the expression for the standard deviation of the bond length of the atomic molecules using harmonic oscillator operator wave faction when it is in it's ground state then calculate the percentage of the equilibrium bond length in this standard deviation for carbon II Oxide (CO) in it ground state (where $C^{12}O^{6}$,$V=2170cm^{-1}$ and Rc=113pm. **[5marks]**

QUESTION FIVE (20 MARKS)

a) State three modes of motion **[3 marks]**

b) Calculate the most probable radius r at which an e- will be found when it occupies a 1s orbital of a hydrogenic atom of atomic number Z and tabulate values1e- species from H to Ne. **[8 marks]**

c) Show that e^{ax} is an *Eigen* function of the operator d/dx and find corresponding Eigen value.

Also show that e^{ax2} is non an eigen function of the same operator **[6marks]**

d) Draw the schematic diagram for the lowest energy molecularorbitals of Homo-nuclear diatomic molecules **[3 marks]**

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